# Hydromechanical couplings in the clay matrix of argilite: some methodological aspects of the atomistic-to-continuum upscaling (poster)

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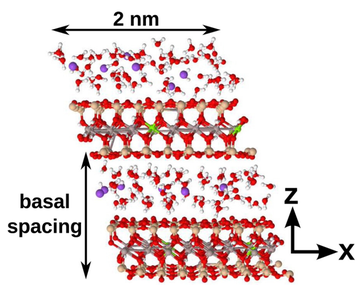
## Context

- Clays are ubiquitous in civil engineering applications
- Good knowledge of their mechanical behaviour is necessary
- Swelling clays are highly sensitive to relative humidity
- Hydromechanical couplings *must* be accounted for $\sigma = f(\varepsilon, RH)$

## Aim of this study

- Modelling of hydromechanical couplings in the clay matrix of argilite
- Investigation of the influence of local orientational order

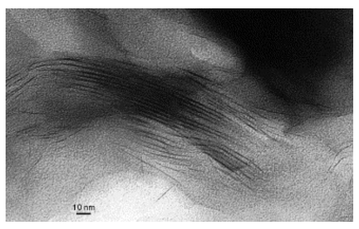
## Numerical, multi-scale approach




### Microscopic scale : the clay sheet

- Molecular dynamics (μVT and NΣT)
- Models developed by Carrier
- Uses theoretical model of Brochard et al. (2012)

**Brochard (2012)**, JMPS **60(4)**, 606
**Carrier (2013)**, PhD Thesis, Université Paris-Est
**Carrier et al. (2014)**, J. Phys. C **118(17)**, 8933




### Mesoscopic scale : the clay particle

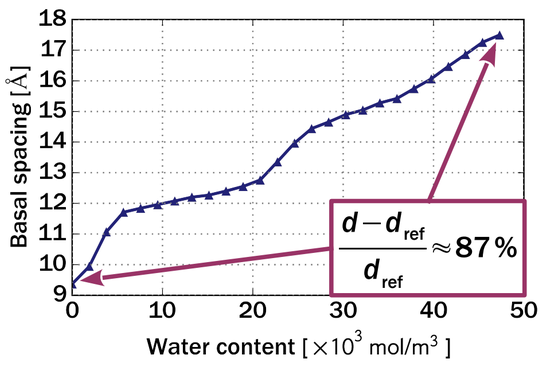
- Rheological models
- Particle viewed as a stack of sheets

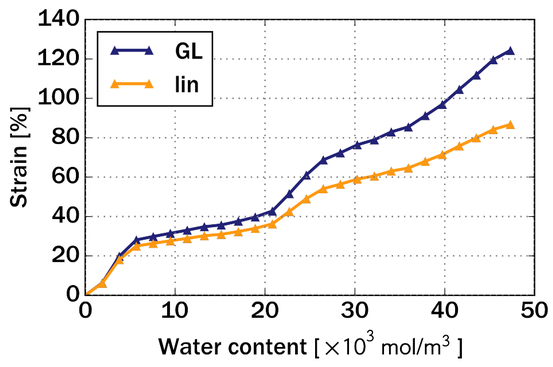
### Macroscopic scale : the clay matrix

- Viewed as a polycrystal
- FFT-based homogenization methods

**Brisard and Dormieux (2010)**, Comp. Mat. Sci. **49(3)**, 663
**Brisard and Dormieux (2012)**, CMAME **217-220**, 197

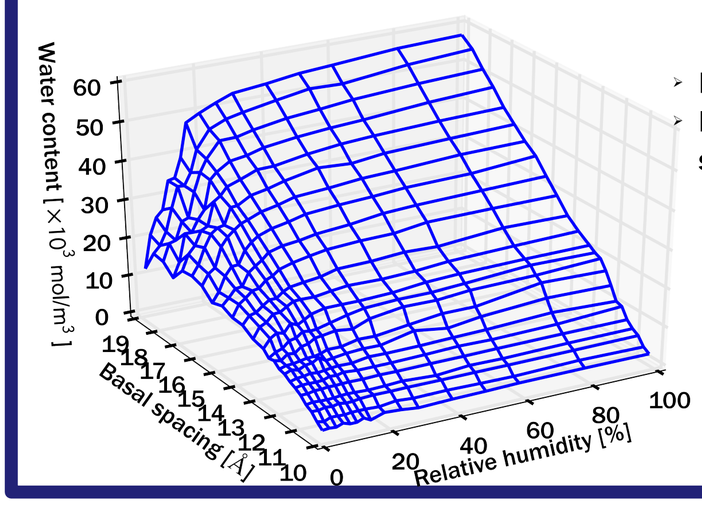
## Finite strains induced by changes in RH




Green-Lagrange strain $E = \frac{d - d_{ref}}{d_{ref}} + \frac{1}{2}\left(\frac{d - d_{ref}}{d_{ref}}\right)^2$

## Adsorption isotherms (from B. Carrier, *op. cit.*)




- Extensive dataset is available
- Derivation w.r.t. *RH*, *d* not trivial due to statistical errors: work in progress!

## Finite strains formulation of molecular simulations

- How to make sure that molecular simulations return the "right" stiffness?
- Need to understand how NΣT simulations are run
- Change of geometry of the unit-cell is accepted with probability

$E_{old}$ strain in the old configuration (measured)

$E_{new}$ strain in the new configuration (measured)

$S$ stress (imposed)

$$p \propto \exp\left(-\frac{S(E_{new} - E_{old})}{kT}\right)$$

This is an energy change!

- Like in mechanics, S is dual to E.
- The nature of S depends on how we measure E.
- If we measure a GL strain, then S is the Piola II stress.

## On the reference configuration

- Strains are measured with respect to a reference configuration
- The stress-free configuration is not unique (depends on the water content)
- Prestressed reference configuration

$$S = C_u(n)\left(E - E_0(n)\right)$$

$E_0(n)$: Free hydric strain

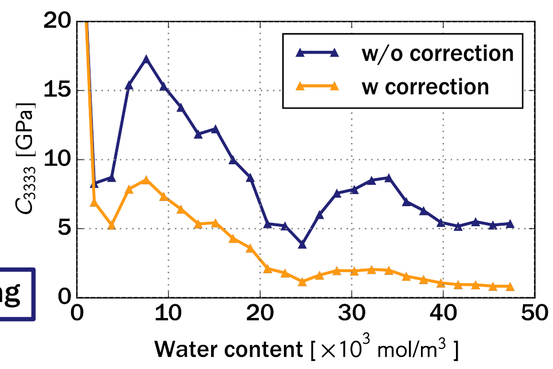
$C_u(n)$: Undrained stiffness

- Correction of molecular dynamics results

$$C_u(n) = \left(\frac{d_{ref}}{d_0(n)}\right)^4 \widetilde{C}_u(n)$$

$\widetilde{C}_u(n)$: Direct output of MD

$d_0(n)$: Stress-free basal spacing



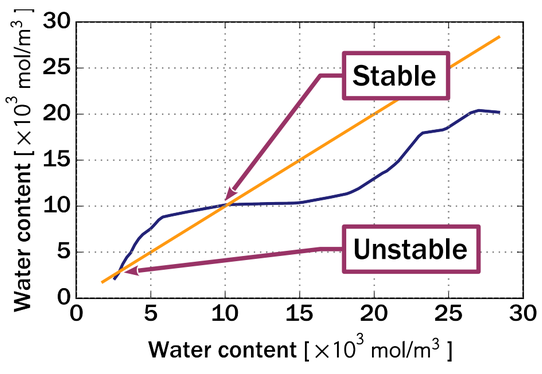

## Undrained vs. drained stiffness

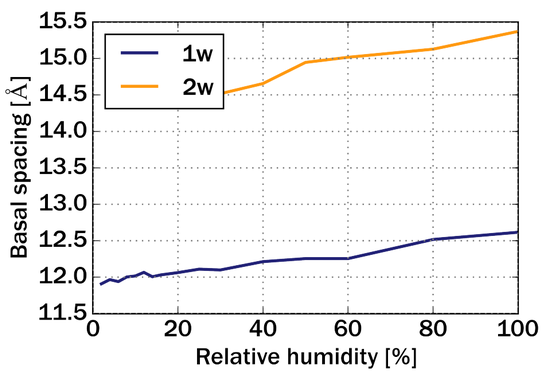
- In our MD simulations, the water content is fixed: undrained stiffness $C_u(n)$
- In the continuum mechanics simulations (at the scale of the clay matrix), we control the relative humidity (or chemical potential of water): drained stiffness $C_d(\mu)$
- We need to perform a change of state variables $(E, n) \rightarrow (E, \mu)$

$$C_d(\mu) = C_u(n) - \left(\frac{\partial n}{\partial \mu}\right)^{-1}\left(\frac{\partial n}{\partial E}\right)^2$$

- Requires the adsorption isotherm $n(d, \mu)$ and its derivatives!

## Application: stable equilibria at fixed relative humidity




Fixed-point equation $n_{MC}(d_0(n), \mu) = n$


## Acknowledgements

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